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THEORETICAL AND EXPERIMENTAL STUDIES IN ASTROPHYSICS

Prepared by:

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CONTENTS

1: INTRODUCTION

The overall research programme of the Molecular Excitation Group in the Department of Physics at the University of Western Ontario is in the broad field of Laboratory Astrophysics. The theoretical and experimental aspects of the programme attempt to provide basic information (such as wavelengths, transition arrays, transition probabilities etc.) on atomic and molecular species of importance in astrophysics and in aeronomy, and also to study their reaction and excitation mechanisms.

This report is similarly arranged to the first semi-annual report.

2: SYNOPSIS OF GENERAL RESEARCH PROGRAMME

2.1 Experimental

2.1.1 Intensity Measurements on Molecular Spectra ($\lambda\lambda$1000A-3μ)

2.1.2 General Molecular Spectroscopy of Electronic Band Systems

2.1.3 Atlas of Molecular Spectra

2.1.4 Shock Tube Spectroscopy

2.1.5 Plasma Jet Studies

2.1.6 Electron Beam Spectroscopy

2.1.7 Ion Beam Spectroscopy

2.1.8 X-Radiolysis of Gases

2.1.9 Ablation Studies

2.1.10 Impact Flash Spectroscopy

2.1.11 Laser Excitation of Powdered Solids

2.2 Theoretical

2.2.1 Molecular Potentials and Vibrational Wavefunctions

2.2.2 Franck-Condon Factors and r-Centroids

2.2.3 Vibration-Rotation Interaction

2.2.4 Atomic Collisions

3: PERSONNEL

The personnel of the research group has changed a little during this report period compared to the previous period. Drs. Marr, Brocklehurst and Hébert returned to their respective Universities at the end of the summer although Dr. Hébert visited us in a consulting capacity in mid-December. A number of new graduate students have joined the group, Miss Haycock completed the requirements for her Master's degree and left the group. Mr. Koehler a graduate technical assistant until August became a graduate student in September 1963.

Faculty

Dr. R. W. Nicholls, Senior Professor of Physics (Director)

Dr. H. I. S. Ferguson, Associate Professor of Physics (Assoc. Director, Experimental)

Dr. P. A. Fraser, Professor of Physics (Assoc. Director, Theoretical)

Dr. G. S. Rose, Assistant Professor of Physics (Plasma Studies)

Dr. R. C. Murty, Assistant Professor of Physics (Molecular Spectroscopy)

Mr. W. R. Jarmain, Lecturer in Physics (Theoretical Studies)

Visiting Professors (Summer 1963)

Dr. G. V. Marr, Lecturer in Physics, University of Reading, England.

Dr. B. Brocklehurst, Lecturer in Chemistry, University of Sheffield, England.

Dr. G. R. Hébert, Assistant Professor, Physics, St. Francis Xavier University, Nova Scotia.

Post-Doctoral Fellow

Dr. D. C. Tyte, National Research Council of Canada Post Doctoral Fellow.

Graduate Students (Supported by scholarship where indicated)

Mr. V. Degen

Mr. N. A. Doughty (Commonwealth Scholarship)

Mr. J. P. Fallona (Ontario Scholarship)

Miss S. Haycock (NRC Scholarship)

Mr. R. A. Koehler (Canadian Kodak Co., Graduate Fellowship 1963-64)

Mr. M. Kraidy

Miss I. S. Lee (Ontario Scholarship)

Mr. R. P. Lowe (DRB on leave)

Mr. J. Mentall

Mr. D. McEwen (DRB on leave)

Mr. A. McGregor (NRC Scholarship)

Mr. F. Morgan (NRC Scholarship)

Mrs. M. Murty

Graduate Technical Assistants

Mr. W. Doan (Summer 1963)

Technician

Mr. J. Radema

Secretary

Mrs. D. Sass

4: SPECIFIC RESEARCH ACTIVITIES

4.1 Experimental

4.1.1 Intensity Measurements on Molecular Spectra

Drs. D. C. Tyte and G. R. Hébert have completed their intensity measurements on the AlO band system and a paper on this work is in press in the Proceedings of the Physical Society. Dr. G. V. Marr completed his theoretical study of the electronic transition moment variation of the O_2 Schumann-Runge and NO Beta and Gamma band systems and two papers on this work are in press in the Proceedings of the Physical Society and in the Canadian Journal of Physics. Dr. Nicholls made a study of transition probability parameters of aeronomical importance which was presented at the aeronomy symposium at the International Union of Geodesy and Geophysics meetings in Berkeley in August. A paper summarising this is in press in Annales de Géophysique. Mr. D. McEwen continues his photoelectric intensity measurements in the vacuum ultraviolet on a number of band systems of N_2, N_2^+, NO, CO and CO^+ of importance in planetary atmospheres and is developing a method of using Cerenkov radiation both

from radio-active sources and also from the electron microtron in the department as the means of calibrating his detectors in the wavelength range 1000-2000A. Mr. V. Degen has commenced experimental work to measure intensities of the O_2^+ first negative and O_2 Herzberg band systems which are both of aeronomical importance. Dr. Murty has commenced experimental studies on vibration-rotation interaction on OH.

4.1.2 General Molecular Spectroscopy of Electronic Band Systems

Mrs. Murty and Dr. Nicholls continue their studies of vibrational intensity distributions of molecular spectra.

4.1.3 Atlas of Molecular Spectra

Scientific reports (one per band system) are being prepared as part of a general atlas of diatomic molecular spectra of importance in aeronomy and astrophysics. Reports are in preparation for the O_2 Schumann-Runge band system (Dr. Hebert, Dr. Marr), CN Red and CN Violet band systems (Dr. Brocklehurst), CO band systems (Mrs. Murty, Dr. Nicholls), N_2 and N_2^+ band systems (Dr. Tyte), AlO band systems (Drs. Tyte and Hebert).

4.1.4 Shock Tube Spectroscopy

Oscillator strength measurements are being made on shock excited MgH by Mr. McGregor. During the report period he has significantly improved his shock tube and peripheral equipment, developed a blast shutter for the spectrograph, and made computer studies of the predicted gas dynamic behaviour of the shock tube which he finds agrees with the experimental behaviour very well. Dr. Tyte and Mr. McGregor have also been studying shock excited TiO and UO band systems which are probably of importance in stellar envelopes. Dr. Tyte and Mr. Radema have completed construction and testing of a new 3 inch diameter 40 ft. long shock tube for which the comprehensive electronic instrumentation described in the previous report was constructed. During the past month preliminary spectroscopic studies of shock excited powdered metallic oxides have commenced.

4.1.5 Plasma Jet Studies

Mr. Morgan continues his concurrent optical and electrical studies of a Mach 3 plasma jet in argon.

4.1.6 Electron Beam Spectroscopy

No work has been done on this project during the report period.

4.1.7 Ion Beam Spectroscopy

Mr. Lowe and Dr. Ferguson continue their studies on spectroscopic aspects of stopping power in 40 KeV proton beams and in 2-8 KeV Na^+, Li^+, Cs^+, K^+ beams in a variety of target gases.

Technical improvement of the 100 KeV proton accelerator arrangement has occupied most of the report period.

A considerable amount of new spectral survey work has been done from the alkali ion accelerator. The results of which were presented by Mr. Lowe at the Sixteenth Gaseous Electronics Conference in Pittsburgh, October 1963.

4.1.8 X-Radiolysis of Gases

Miss Lee has been making a quantitative spectroscopic study of the very feeble light emitted when 60 KV Cu x-rays pass through a N_2, O_2, H_2, He and air. She has been studying the variation of intensity of spectral features as a function of gas pressure and x-ray dosage using a Cerenkov radiation source to calibrate her film. The fluorescent efficiencies of the gases are being studied also.

4.1.9 Ablation Studies

Mr. Koehler, Mr. Radema and Dr. Nicholls are studying ablation phenomena in shock excitation of powdered metals and also in the interaction between high speed wax pellets and the atmosphere through which they travel.

4.1.10 Impact Flash Spectroscopy

Mr. Koehler and Dr. Nicholls are making spectroscopic studies of 1 microsecond duration flashes which occur when high speed (5000f/s) pellets impact on metal targets.

4. 1. 11 Laser Excitation of Powdered Solids

Mr. Mentall and Dr. Nicholls have followed an earlier qualitative survey by a systematic research programme on laser excitation of powdered solids somewhat similar to the research programme of the past few years on the shock excitation of powdered solids.

4. 2 Theoretical

4. 2. 1 Molecular Potentials and Vibrational Wavefunctions

Mr. Jarmain and Dr. Nicholls have completed their study of the continuum wavefunctions above the dissociation limit of the $B^3\Sigma$ state of O_2 and have recently completed a semi-theoretical study of the intensity distribution of the Schumann-Runge photodissociation continuum. A paper on this work is in preparation. They have recently commenced study on a similar photodissociation continuum of the O_2 Herzberg band system. Mr. Jarmain is also continuing his calculations on the realistic Franck-Condon factors of more bands of the O_2 Schumann-Runge system.

4. 2. 2 Franck-Condon Factors and r-Centroids

Dr. Nicholls has continued his computation in Franck-Condon factor arrays of many band systems of astrophysical and aeronomical importance to high vibrational quantum numbers based on a Morse model. Those recently studied and as yet unpublished are listed in the table below. Dr. Nicholls and Mrs. Murty have been making fundamental theoretical studies of the geometry in the $v'v''$ plane of Condon loci. Dr. Nicholls has found a method of interpolation between Franck-Condon factor tables.

TABLE I

Transitions for which Franck-Condon factor arrays have been computed since the previous report

H_2	Lyman	OH	Violet
MgH	A-X	O_2	Herzberg I
	C-X		Herzberg II
	C-A		Herzberg III
I_2	B-X		Chamberlain
O_2^+	1st Negative		Noxan
	2nd Negative		I. R. Atmospheric
CN	Red		Atmospheric
	Violet		Broida-Gaydon
C_2	Swan	NO	γ
	Fox Herzberg		β
	Phillips		δ
	Deslandres-D'Azambuja		ϵ
	Mulliken		γ'
	Balik-Ramsay		β'
BN	Violet		M
$O_2(X)$	O_2^+ (X, A, a, b)		Feast 1
ZrO	C-X		Feast 2
	B-X		Ogawa 1
	A-X		Ogawa 2
	b-a	NO^+	A-X
	d-c	NO (X) $\rightarrow$	NO^+ (A, X)

4. 2. 3 Vibration-Rotation Interaction

Professor Fraser and Miss Haycock (M. Sc. thesis 1963) have extended some earlier work of Professor Fraser on the effect of the molecular rotation in vibrational intensities and have obtained tabulated and graphical results for OH, OD and MgH in particular. The effect appears to be not inconsiderable for hydrides and should be experimentally measureable (by comparison of band profiles) in MgH.

4. 2. 4 Atomic Collisions

Professor P. A. Fraser and his students Mr. N. A. Doughty, Mr.

M. Kraidy and Mr. R. P. McEachran (a post-doctoral fellow at University College London, England during the report period) have been working collaboratively on a number of separate though connected problems on electron-hydrogen elastic scattering. The work may be summarized as follows:

Electron-Hydrogen Collisions (Professor Fraser and Dr. McEachran)

The work on elastic collisions of electrons by hydrogen atoms for electron energies insufficient to excite the atoms was completed (except for the singlet S-wave where for some energies convergence difficulties prevailed) in the 1s-2s-2p approximation on the IBM 7090 computer at the National Bureau of Standards, Washington. This work was described in the Ph. D. thesis (1962) of Dr. McEachran and has been published in the Proceedings of the Physical Society 82, 1038, 1963. The results confirm generally those of Burke and Schey (referred to in the previous annual report) for the same calculation, with a perhaps significant difference near the threshold in the singlet L = 1 state.

The computer code is being generalized to include up to the 3d state of H in the eigenfunction expansion, and to treat problems above threshold energies. The integral equation methods used are ideally suited for the R-matrix calculations for inelastic collisions. Methods of speeding convergence of the iterative methods are being investigated, as well as methods of obtaining convergence, e. g. for the singlet S-wave (see below). Adaptation of the code for the case of collisions with H-like ions has begun. At the request of Professor Spruch of New York University, some positron collision calculations have been performed with this code, to aid his work. Further, a detailed search was made for new resonances reported informally by Burke and Schey and none were found.

Photobinisation of H^- (Professor Fraser and Mr. Doughty)

The 1s-2s-2p singlet P-wave results described above have been used in a calculation of the bound-free absorption coefficient of H^-. Schwartz'

function for H^- gave the best results; the Hylleraas type function of Hart and Herzberg was also used. As found by Geltman, the use of the Schwartz function gives a significant improvement to the result using the length operator. The agreement between the results using the length, velocity and acceleration forms of the operator was not perfect, but satisfying. The work has been reported upon (Doughty and Fraser, Proceedings of the Third International Conference on The Physics of Electronic and Atomic Collisions, London, England, July 1963, in press). The bound-free calculation is being extended to include the singlet P-wave 1s-2s-2p-3s-3p-3d free functions from the work of McEachran and Fraser. Further a calculation of the free-free transition of an electron in the field of a hydrogen atom is proceeding using these free waves for both spin states and all significant values of L. This work has largely been done on the IBM 7090 computer at the University of Toronto though some preliminary work was done at the National Bureau of Standards and also in the computing centre at the University of Western Ontario.

Computation Methods (Professor Fraser and Mr. Kraidy)

A promising technique of obtaining convergence and of speeding convergence in the integral equation iteration method is being investigated. While the previous method was designed to converge to the tangent of the phase-shift, the new method is designed to converge to the cotangent. It can be generalized to inelastic problems to give the M-matrix rather than the R-matrix. The method has been applied with success to some elementary square well interaction problems, and is now being applied to the singlet S-wave e-H problem. After their full development, these methods will be incorporated into the main e-H computer code.

Variation-iteration methods suggested by Saraph and Seaton, and by Saraph, for the tangent of the phase shift and for the R-matrix are being developed and adapted for use with the cotangent of the phase shift and the M-matrix. These methods should greatly cut down upon the number of iterations required in a solution.

5: PUBLICATIONS

5.1 Published Papers

The following papers arising from the research programme appeared in the literature during the report period.

Electrical and optical studies of the argon plasma jet
Cana dian Journal of Physics 41, 1405-1419, 1963
M. D. Watson, H. I. S. Ferguson and R. W. Nicholls.

The spectroscopy of shock excited powdered solids
Applied Optics 2, 919-930, 1963
R. W. Nicholls, W. H. Parkinson and E. M. Reeves.

Effect of Virtual excitation of the 2s and 2p states on the elastic scattering of electrons by atomic hydrogen
Proceedings of the Physical Society 82, 1038, 1963
R. P. McEachran and P. A. Fraser.

Franck-Condon factors from Klein-Dunham potentials for bands of the Schumann-Runge system of O_2
Canadian Journal of Physiss 41, 414-416, 1963
W. R. Jarmain.

Primary and Subsidiary Condon loci of molecular spectra
Nature 199, 794, 1963
R. W. Nicholls.

Franck-Condon factors from Klein-Dunham potentials for the v''=0 progression of the Schumann-Runge system of O_2
Canadian Journal of Physics 41, 1926-1929, 1963
W. R. Jarmain.

Research and Canadian Industry
The Business Quarterly 28, 12-29, 1963
R. W. Nicholls.

"Line Intensities in diatomic electronic spectra, The Effect of vibration-rotation interaction"
M. Sc. Thesis 1963
Miss Shirley A. Haycock.

5.2 Papers Submitted to Journals

The following papers have been submitted to journals and are in press.

Electronic transition moments and their effects on the band strengths and absorption oscillator strengths of the NOβ andγ systems
Proceedings of the Physical Society (In Press)
G. V. Marr.

The Electronic transition moment for the O_2 Schumann-Runge band system of O_2
Canadian Journal of Physics (In Press)
G. V. Marr.

Transition probabilities of aeronomically important spectra
Annales de Geophysique (In Press)
R. W. Nicholls.

Intensity measurements on the $A^2\Sigma$-$X^2\Sigma$ system of AlO
Proceedings of the physical Society (In Press)
G. R. Hebert and D. C. Tyte.

Laboratory Astrophysics and combustion spectroscopy
AGARDOGRAPH (In Press)
R. W. Nicholls.

Franck-Condon factors to high vibrational quantum numbers III: CN
Journal of Research of the National Bureau of Standards (In Press)
R. W. Nicholls.

5.3 Orally Presented Papers

The following papers were orally presented at the scientific meetings indicated.

"Transition probabilities of aeronomically important spectra"
R. W. Nicholls.
Invited paper to Aeronomy Symposium, International Union of Geodesy and Geophysics Congress, Berkeley California, August 28, 1963.

"Optical excitation of gases by alkali ion bombardment"
R. P. Lowe and H. I. S. Ferguson.
16th Gaseous Electronics Symposium of American Physics Society
Pittsburgh, P. A., October 16-18, 1963.

"Condon loci in molecular spectra"
Mrs. M. Murty.
Tri-University Colloquium, University of Buffalo, October 1963.